Statistical and Thermal Physics: Homework 14

Due: 27 March 2020

1 Ensembles of spin-1/2 particles

Consider an ensemble of 16 spin-1/2 particles. There is no magnetic field present.

a) List the possible macrostates of the ensemble.

b) Determine the total number of microstates possible.

c) Determine the number of microstates that are associated with each of the macrostates. Your answer should be a list and you can use a calculator or Excel to compute the numbers.

d) How does the probability of attaining the microstate

$$\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow$$

compare to the probability of attaining the microstate

$$\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow?$$

Explain your answer.

e) Determine the probability with which each macrostate could occur.

f) Which macrostate is most probable?

g) What is the probability that a macrostate will contain *at least* 4 spin up particles?

h) What is the probability that a macrostate will contain *at most* 5 spin up particles?

2 Accessible and inaccessible microstates

Consider a system of non-interacting spin-1/2 particles. The energy of a single particle with spin up is $-\mu B$ and that with spin down is μB. If the total energy of the system is fixed, then an accessible microstate is one that gives this total energy. Suppose that the system consists of six particles and that the total energy of the system is $-2\mu B$.

a) Describe which macrostates are possible in terms of the number of particles with spin up.

b) List all accessible microstates.

c) Determine the probability with which on particular given particle (e.g. the leftmost) will be in a state with spin up.

d) Determine the probability with which any two given particles will be in states with spin up.

3 Ensembles of spin-$1/2$ particles in a magnetic field: small number example

The energy of a particle with spin up in a magnetic field with magnitude B oriented along the positive z axis is $-\mu B$. That for a particle with spin down is μB. Consider an ensemble of eight spin-1/2 particles in this field. Assume that the probability with which a particle is in the spin up state is 3/4 and the probability that it is in the spin down state is 1/4. Let N_+ represent the number of particles with spin up.

a) List all macrostates for the ensemble (in terms of N_+), the energy of each macrostate and the probability with which each occurs.

b) Which is the most likely macrostate? With what probability does it occur?

c) Determine the mean for the energy, $\overline{E}$ (this is for a large collection of such ensembles). Is there a macrostate which has an energy exactly equal to the mean energy?

d) Determine the standard deviation for the energy, σ_E.

e) Suppose that one is given a single copy of ensemble without knowing its actual microstate. One way to assign an energy to it is to use the mean energy. What is the probability that the ensemble's microstate is that whose energy is exactly the mean energy?

It should be clear that the ensemble could be in a different macrostate. Consider the *two other* macrostates with energy closest to that of the mean energy.

f) List the energies of these macrostates and determine the fractional difference between the energies of these and the mean energy.

g) Determine the probability that the ensemble could have either the mean energy or one of the two other energies that are closest to the mean energy.

h) Determine the probability that the ensemble could have an energy in the range $\overline{E} - \sigma_E$ to $\overline{E} + \sigma_E$.

i) Based on the previous results you should be able to make a statement of the form: "The energy of the ensemble is within ??% of the mean with probability =??." Provide such a statement or statements for this example.

4 Ensembles of spin-$1/2$ particles in a magnetic field

The energy of a particle with spin up in a magnetic field with magnitude B oriented along the positive z axis is $-\mu B$. That for a particle with spin down is μB. Consider an ensemble of N spin-1/2 particles in this field and assume that N is even. Let N_+ represent the number of particles with spin up. The probability with which any given particle will be in the spin up state is different to that in which it will be in the spin down state. It will emerge that the spin up state is favored over the spin down state. Denote the probability with which any particle is in the spin up state by $(1+\varepsilon)/2$ where $0 \leqslant \varepsilon \leqslant 1$.

a) Show that,

$$\overline{E} = -\mu B N \varepsilon$$

and that the standard deviation of the energy, .

$$\sigma_E = \mu B \sqrt{(1 - \varepsilon^2)N}.$$

b) Show that the magnitude of the ratio of the standard deviation to the mean approaches zero as the size of the ensemble increases.

In order to illustrate these consider numerical examples for which $\mu B = 1/2$ and $\varepsilon = 1/3$. The aim will be to determine the probability with which the energy of a macrostate is within the range of a standard deviation of the mean.

c) Show that $\overline{E} = -N/6$ and $\sigma_E = \sqrt{2N/9}$. Show that the value of N_+ that gives the macrostate with energy exactly equal to $\overline{E}$ is $N_+ = 2N/3$. Show that the value of N_+ that gives the macrostate with energy exactly equal to $\overline{E} \pm \sigma_E$ is $N_+ = 2N/3 \mp \sqrt{2N/9}$.

In each of the following you can use a numerical tool (e.g. Excel) to do the computations. These all concern the range of the energies $\overline{E} - \sigma_E$ to $\overline{E} + \sigma_E$, A measure of this range is the ratio $|\sigma_E/\overline{E}|$.

d) Let $N = 21$. Determine $|\sigma_E/\overline{E}|$. Determine the probability with which the energy of a macrostate is in the range $\overline{E} - \sigma_E$ to $\overline{E} + \sigma_E$.

e) Let $N = 90$. Determine the fractional difference between the mean energy $\overline{E}$ and the extremes of the energies in the range $\overline{E} - \sigma_E$ to $\overline{E} + \sigma_E$. Determine the probability with which the energy of a macrostate is in the range $\overline{E} - \sigma_E$ to $\overline{E} + \sigma_E$.

f) Let $N = 150$. Determine the fractional difference between the mean energy $\overline{E}$ and the extremes of the energies in the range $\overline{E} - \sigma_E$ to $\overline{E} + \sigma_E$. Determine the probability with which the energy of a macrostate is in the range $\overline{E} - \sigma_E$ to $\overline{E} + \sigma_E$.

g) Does the range of energies $\overline{E} - \sigma_E$ to $\overline{E} + \sigma_E$ become more precise, relative to the mean energy, as N increases?

h) Does the probability of falling within the range energies $\overline{E} - \sigma_E$ to $\overline{E} + \sigma_E$ become larger or smaller as N increases? Does it appear to approach a fixed value?

5 Einstein solid statistics: small numbers

Consider an Einstein solid consisting of five particles (these are labeled A, B, C, D and E).

a) Determine the multiplicities for the four lowest energy states.

b) Suppose that there are three energy units. Determine the probability with which one particle will have all three energy units.

c) Suppose that there are three energy units. Determine the probability with which particle 1 has two energy units.

6 Einstein solid statistics: large numbers

Consider two Einstein solids, labeled A and B. Solid A has 10 particles and solid B has 10 particles. The exercise will consider various energy units. Calculations can be done using the OSP program called Einstein solid: temperature. Suppose that initially the energy number for A is $q_A = 9$ and, for B, $q_B = 3$. In the following do not forget the $\hbar\omega$ and $N/2$ terms in teh energy.

a) Determine the multiplicities Ω_A and Ω_B. Determine the total number of microstates for the composite system. Determine the energy per particle for each solid.

b) Now suppose that the systems can interact, exchange energy and eventually reach equilibrium. Use the program to determine and describe the most probable state for each solid. Determine the the energy per particle for each solid.

c) In what direction did the energy flow as the systems approached equilibrium?

d) Determine the probability that the energy flows from system A to system B. Determine the probability that the energy flows from system B to system A. How many times is it more likely that energy flows from A to B rather than from B to A?

Now suppose that solid A initially has 20 particles and $q_A = 20$ while solid B has 5 particles and $q_B = 10$.

e) Determine the equilibrium state after the solids have interacted. Determine the energy per particle for each solid.

f) Did the energy flow from the solid with higher total energy to that with lower total energy?

2020 HW14 Q1

a) Macrostates can be labeled by the number of spin up particles, N_+. Then

$N_+ = 0, 1, 2, 3, 4, \ldots, 15, 16$

b) Each particle can be in one of two states. Thus there are

$\frac{1}{2} \times \frac{1}{2} \times \ldots \times \frac{1}{2} = \frac{1}{2^{16}} = 65536$

states

c) The number of microstates associated with macrostate N_+ is

$$\binom{N}{N_+} = \frac{N!}{N_+ (N-N_+)!}$$

N_+	number	prob
0	1	0.000015
1	16	0.00024
2	120	0.00183
3	560	0.00854
4	1820	0.02777
5	4368	0.06665
6	8008	0.12219
7	11440	0.17456
8	12870	0.19638
9	11440	0.17456
10	8008	0.12219
11	4368	0.06665
12	1820	0.02777
13	560	0.00854
14	120	0.00183
15	16	0.00024
16	1	0.000015

d) each microstate is equally likely as each spin ½ particle has an equal probability of being in 4 vs 6

These are <u>equally</u> likely.

e) $$p(N_+) = \binom{N}{N_+}\left(\frac{1}{2}\right)^{N_+}\left(\frac{1}{2}\right)^{N-N_+} = \frac{1}{2^N}\binom{N}{N_+}$$

See table in (c)

f) $N_+ = 8$

g) This is $p(N_+ = 4) + p(N_+ = 5) + \dots + p(N_+ = 16)$

From the table this is $\boxed{0.98937}$

h) This is $p(N_+ = 0) + p(N_+ = 1) + \dots + p(N_+ = 5) = \boxed{0.10506}$

2020 HW 14 Q2

a) $E = n_+(-\mu B) + n_-(\mu B)$ where $n_+ =$ number up

$n_- =$ number down

$= -\mu B(n_+ - n_-)$

Then $n_- = N - n_+ \Rightarrow E = -\mu B(2n_+ - N)$

We need $E = -2\mu B = -\mu B(2n_+ - N)$

$\Rightarrow 2 = 2n_+ - N$

$\Rightarrow n_+ = \frac{2+N}{2}$

Here $N = 6 \Rightarrow n_+ = 4$. The states are

b)

↑↑↑↑↓↓	↓↑↑↑↑↓
↑↑↑↓↑↓	↓↑↑↑↓↑
↑↑↑↓↓↑	↓↑↑↓↑↑
↑↑↓↑↑↓	↓↑↓↑↑↑
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↑↓↓↑↑↑	

There are $\binom{6}{2} = \frac{6!}{4!\,2!} = 15$ states

1c) Look at leftmost spin particle. There are 10 ways it can be up.

$$\text{Prob} = \frac{10}{15} = \frac{2}{3}$$

d). Look at leftmost two particles. There are 6 ways they can both be up

$$\text{Prob} = \frac{6}{15} = \frac{2}{5}$$

2020 HW 14 Q3

a) $E = N_+(-\mu B) + N_-(\mu B)$

$= \mu B(N_- - N_+)$ $\qquad N = N_+ + N_- \Rightarrow N_- = N - N_+$

$= \mu B(N - 2N_+)$

$$\text{Prob}(N_+) = \binom{N}{N_+} p_+^{N_+} p_-^{N_-}$$

$$= \binom{N}{N_+}\left(\frac{3}{4}\right)^{N_+}\left(\frac{1}{4}\right)^{N_-}$$

$$= \left(\frac{1}{4}\right)^{N_+ + N_-}\binom{N}{N_+} 3^{N_+}$$

$$= \left(\frac{1}{4}\right)^{8}\binom{N}{N_+} 3^{N_+}.$$

$$= \frac{1}{65536}\binom{8}{N_+} 3^{N_+}$$

N_+	E	Prob all over 65536	
0	$8\mu B$	1/...	1
1	$6\mu B$	24/...	8
2	$4\mu B$	252/...	28
3	$2\mu B$	1512/...	56
4	0	5670/...	70
5	$-2\mu B$	13608/	56
6	$-4\mu B$	20412/	28
7	$-6\mu B$	17496/	8
8	$-8\mu B$	6561/...	

b) $N_+ = 6 \quad N_- = 2$ $\qquad \text{prob} = \dfrac{20412}{65536} = 0.311$

c) $\bar{E} = \mu B(N - 2\bar{N}_+)$

$= \mu B(8 - 2\bar{N}_+)$ $\qquad$ For binomial $\bar{N}_+ = p_+ N$

$\qquad = \frac{3}{4}8 = 6$

$= \mu B(8 - 12)$

$\bar{E} = -4\mu B$

d) $\sigma_E^2 = \overline{E^2} - \bar{E}^2 = \overline{(\mu B(N-2N_+))^2} - (\mu B(N - 2\bar{N}_+))^2$

$= (\mu B)^2\overline{[N^2 - 4NN_+ + N_+^2]} - (\mu B)^2[N^2 - 4N\bar{N}_+ + 4\bar{N}_+^2]$

$= (\mu B)^2[N^2 - 4N\bar{N}_+ + \overline{N_+^2}] - (\mu B)^2[N^2 - 4N\bar{N}_+ + 4\bar{N}_+^2]$

$$\sigma_E^{\ 2} = (\mu B)^2 \sigma_{N+}^{\ 2}$$

$$= \mu B\ N\ p_+(1-p_+)$$

$$\sigma_E = \mu B \sqrt{8 \ \frac{3 \cdot 1}{16}}$$

$$= \mu B \sqrt{6} \qquad \sigma_E = 2.45\ \mu B$$

e) This is $N_+ = 6 \Rightarrow$ prob $= 0.311$

f) These are

$N_+ = 5 \Rightarrow E = -2\mu B$

$N_+ = 7 \Rightarrow E = -6\mu B$

The diff in energy from $N_+ = 6$ is $2\mu B$

Fractional diff is $\left|\frac{2\mu B}{-4\mu B}\right| = \frac{1}{2}$ frac diff $= 1/2$

g) This is prob $(N_+ = 5)$ + prob$(N_+ = 6)$ + prob$(N_+ = 7) = 0.788$

h) The values of E range the same as for g $\Rightarrow 0.788$

i) The energy is within 50% of $-4\mu B$ with prob 0.788

a) $p_\uparrow = \frac{1+\varepsilon}{2}$

$p_\downarrow = 1 - p_\uparrow = \frac{1-\varepsilon}{2}$

Let N_+ be the number of particles with spin $\uparrow$
N_- " " " " " " " $\downarrow$

Then the energy is

$$E = -N_+ \mu B + N_- \mu B = \mu B (N_- - N_+)$$

$$= \mu B (N - N_+ - N_+)$$

$$E = \mu B (N - 2N_+)$$

Now $\bar{E} = \mu B (N - 2\bar{N}_+)$

and $\bar{N}_+ = N p_\uparrow$

$$\Rightarrow \bar{E} = \mu B \left[N - 2N \left(\frac{1+\varepsilon}{2} \right) \right]$$

$$= \mu B N \left[1 - 1 - \varepsilon \right]$$

$$\Rightarrow \boxed{\bar{E} = -\mu B N \varepsilon}$$

Then $\sigma_E = \sqrt{\overline{E^2} - \bar{E}^2}$ and here

$$E^2 = \mu^2 B^2 (N - 2N_+)^2 = \mu^2 B^2 (N^2 - 4N N_+ + 4N_+^2)$$

$$\overline{E^2} = \mu^2 B^2 (N^2 - 4N \bar{N}_+ + 4\overline{N_+^2})$$

For binomial distributions

$$\overline{N_+} = N p_\uparrow$$

$$\overline{N_+^2} = \overline{N_+}^2 + N p_\uparrow p_\downarrow$$

$$= N^2 p_\uparrow^2 + N \left(\frac{1+\varepsilon}{2}\right)\left(\frac{1-\varepsilon}{2}\right)$$

$$= N^2 \left(\frac{1+\varepsilon}{2}\right)^2 + N\left(\frac{1-\varepsilon^2}{4}\right)$$

So

$$\overline{E^2} = \mu^2 B^2 \left[N^2 - 4N^2\left(\frac{1+\varepsilon}{2}\right) + N^2(1+\varepsilon)^2 + N(1-\varepsilon^2)\right]$$

$$= \mu^2 B^2 \left[\cancel{N^2} - 2N^2 - \cancel{2N^2 \varepsilon} + N^2(\cancel{1} + \cancel{2\varepsilon} + \varepsilon^2) + N(1-\varepsilon^2)\right]$$

$$= \mu^2 B^2 \left[N^2 \varepsilon^2 + N(1-\varepsilon^2)\right]$$

Then $\overline{E^2} - \overline{E}^2 = \mu^2 B^2 \left[\cancel{N^2\varepsilon^2} + N(1-\varepsilon^2) - \cancel{N^2\varepsilon^2}\right]$

$$\Rightarrow \quad \sigma_E = \sqrt{\mu^2 B^2 N(1-\varepsilon^2)}$$

$$\Rightarrow \quad \sigma_E = \mu B \sqrt{N(1-\varepsilon^2)}$$

b) $$\frac{\sigma_E}{\bar{E}} = \frac{\cancel{\mu B}\sqrt{N(1-\epsilon^2)}}{-\cancel{\mu B}\, N \epsilon}$$

$$\left|\frac{\sigma_E}{\bar{E}}\right| = \frac{\sqrt{1-\epsilon^2}}{\sqrt{N}\,\epsilon} \to 0 \quad \text{as } N \to \infty$$

c) $$\bar{E} = -\frac{1}{2} N \frac{1}{3} = -\frac{N}{6}$$

$$\sigma_E = \frac{1}{2}\sqrt{N\frac{8}{9}} = \sqrt{\frac{2N}{9}}$$

In general $E = \mu B (N - 2N_+) = \frac{1}{2}(N - 2N_+)$

We need $E = \bar{E}$

$$\Rightarrow \frac{1}{2}(N - 2N_+) = -N/6$$

$$\Rightarrow N - 2N_+ = -N/3$$

$$\Rightarrow \frac{4N}{3} = 2N_+ \Rightarrow N_+ = \frac{2}{3}N$$

Then the value of N_+ that gives $\bar{E} \pm \sigma_E$ is

$$\frac{1}{2}(N - 2N_+) = -\frac{N}{6} \pm \sqrt{\frac{2N}{9}}$$

$$\frac{N}{2} - N_+ = -\frac{N}{6} \pm \sqrt{\frac{2N}{9}} \Rightarrow N_+ = \frac{2N}{3} \mp \sqrt{\frac{2N}{9}}$$

d) For the probabilities:

g) $$p(N_+) = \binom{N}{N_+} p_\uparrow^{N_+} p_\downarrow^{N-N_+} = \binom{N}{N_+}\left(\frac{2}{3}\right)^{N_+}\left(\frac{1}{3}\right)^{N-N_+}$$

$$= \frac{1}{3^N}\binom{N}{N_+} 2^{N_+}$$

Also $$\left|\frac{\sigma_E}{\bar{E}}\right| = \sqrt{\frac{2N}{9}} \Big/ \frac{N}{6} = \frac{\sqrt{2N}}{N}\frac{6}{3} = 2\sqrt{\frac{2}{N}}$$

N	$\left\lvert \frac{\sigma_E}{\bar{E}} \right\rvert$	prob range of N+	prob
21	0.617	11.8 < N+ < 16.2	0.754
90	0.298	55.5 < N+ < 64.4	0.686
150	0.231	94.2 < N+ < 105.8	0.659

g) Becomes smaller.

h) Gets smaller, maybe approaches fixed value

2020 HW 14 Q5

a) Lowest energy states:

$q = 0, 1, 2, 3$

$$\Omega(N,q) = \binom{N+q-1}{q} = \frac{(N+q-1)!}{(N+q-1-q)!\,q!} = \frac{(N+q-1)!}{(N-1)!\,q!}$$

Here $N = 5 \Rightarrow \Omega(N,q) = \dfrac{(4+q)!}{4!\,q!}$

q	$\Omega(N,q)$
0	1
1	5
2	15
3	35

b) With $q=3$ there are 35 equally likely microstates. Of these the following have one particle with all energy units. Thus

A	B	C	D	E
0	0	0	0	3
0	0	0	3	0
0	0	3	0	0
0	3	0	0	0
3	0	0	0	0

prob = $5/35 = \frac{1}{7}$

c) The microstates are:

$\left.\begin{matrix} 2 & 1 & 0 & 0 & 0 \\ 2 & 0 & 1 & 0 & 0 \\ & & \vdots & & \end{matrix}\right\}$ 4 total

prob = $4/35$

2020 HW 14 Q6

a) $\Omega_A = \binom{N_A + q_A - 1}{q_A} = \binom{19-1}{9} = \binom{18}{9} = 48620$

$\Omega_B = \binom{N_B + q_B - 1}{q_B} = \binom{13-1}{3} = \binom{12}{3} = 220$

$\Omega = \Omega_A \Omega_B = 10696400$

The energy for a system is $E = \hbar\omega(q + N/2)$. So the energy per particle is

$$E/N = \hbar\omega\left(\frac{q}{N} + \frac{1}{2}\right)$$

For A $\quad E_A/N_A = \hbar\omega\left(\frac{9}{10} + \frac{1}{2}\right) \Rightarrow \frac{E_A}{N_A} = \hbar\omega\frac{14}{10} \Rightarrow \boxed{\frac{E_A}{N_A} = \hbar\omega\frac{7}{5}}$

For B $\quad E_B/N_B = \hbar\omega\left(\frac{3}{10} + \frac{1}{2}\right) \Rightarrow \frac{E_B}{N_B} = \hbar\omega\frac{8}{10} \Rightarrow \boxed{\frac{E_B}{N_B} = \hbar\omega\frac{4}{5}}$

b) The most probable has $q_A = 6 \Rightarrow q_B = 6$

Then for A $\quad E_A/N_A = \hbar\omega\left(\frac{6}{10} + \frac{1}{2}\right) = \hbar\omega\frac{11}{10} \Rightarrow \boxed{\frac{E_A}{N_A} = \hbar\omega\frac{11}{10}}$

Similarly for B - - - - - - - $\Rightarrow \boxed{\frac{E_B}{N_B} = \hbar\omega\frac{11}{10}}$

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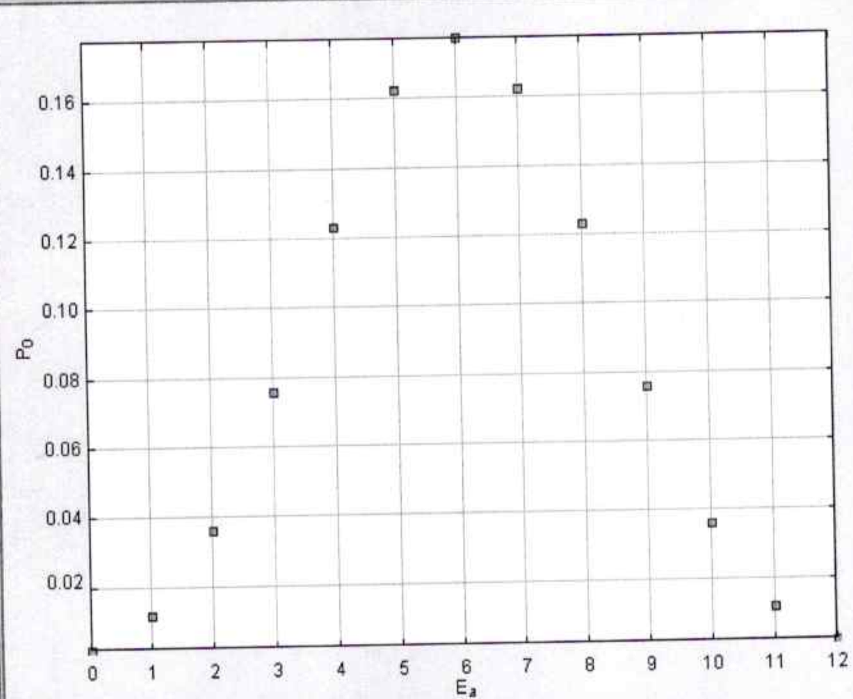

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row	E_a	P_0
0	0	0.002
1	1	0.012
2	2	0.036
3	3	0.076
4	4	0.123
5	5	0.162
6	6	0.178
7	7	0.162
8	8	0.123
9	9	0.076
10	10	0.036
11	11	0.012
12	12	0.002

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c) It flowed from system A to system B

(one with most energy per particle to one with least energy per particle)

d) Prob $(A \to B) =$ Prob (A energy decreases)

$= \text{Prob}\,(q_A = 0) + \text{Prob}\,(q_A = 1) + \cdots + \text{Prob}\,(q_A = 8)$

$= 0.002 + 0.012 + \cdots + 0.123$

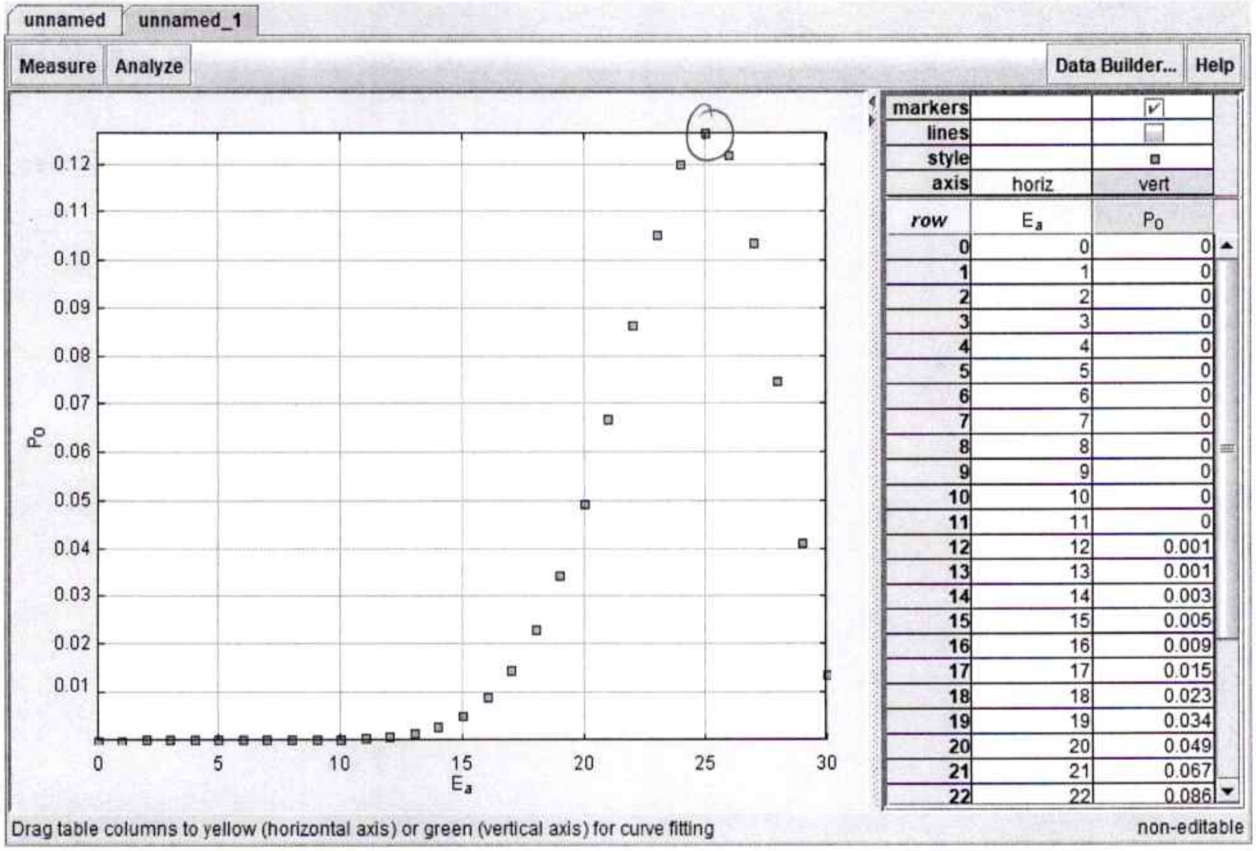
$= 0.874$

Prob $(B \to A)$ = Prob (A energy increases)

$= \text{Prob}(q_A = 10) + \text{Prob}(q_A = 11) + \text{Prob}(q_A = 12)$

$= 0.050$.

e)



Most probable $q_A = 25$ $\left(q_B = 30 - 25 = 5 \right.$

energy $E_A = \hbar\omega(q + N_A/2) = \hbar\omega(25+10) = \hbar\omega 35$ $\quad E_B = \hbar\omega(5+5)$

$E_A/N_A = \hbar\omega \frac{35}{20} = \hbar\omega\, 7/4$ $\quad E_B/N_B = \hbar\omega\, 2$

f) Energy flowed from B → A So <u>not</u> from higher → lower energy

It flowed from higher energy per particle (B) to lower energy per particle (A).